Spontaneous breaking of the Fermi surface symmetry in the $t-J$ model: a numerical study

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We present a variational Monte Carlo (VMC) study of spontaneous Fermi surface symmetry breaking in the $t-J$ model. We find that the variational energy of a Gutzwiller projected Fermi sea is lowered by allowing for a finite asymmetry between the x- and the y-directions. However, the best variational state remains a pure superconducting state with d-wave symmetry, as long as the underlying lattice is isotropic. Our VMC results are in good overall agreement with slave boson mean field theory (SBMFT) and renormalized mean field theory (RMFT), although apparent discrepancies do show up in the half-filled limit, revealing some limitations of mean field theories. VMC and complementary RMFT calculations also confirm the SBMFT predictions that many-body interactions can enhance any anisotropy in the underlying crystal lattice. Thus, our results may be of consequence for the description of strongly correlated superconductors with an anisotropic lattice structure.

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I. INTRODUCTION

The phenomenon of high temperature superconductivity has led to intensive debates about possible superconducting states in purely repulsive models, such as the single band Hubbard model in two dimensions. Various strong coupling approaches show that a repulsive onsite (Hubbard) interaction U may lead to instabilities of the two-dimensional (2D) Fermi sea, such as antiferromagnetism, d-wave superconductivity *etc.* An interesting possibility is the tetragonal symmetry breaking of the 2D Fermi surface due to strong electron correlations, which may result in a quasi one-dimensional (1D) state. This instability, which competes with, and seems to be suppressed by the d-wave pairing state, was first reported by Yamase and Kohno within slave boson mean field theory (SBMFT) in the $t-J$ model.[1] The same effect was seen within a renormalization group (RG) study in the Hubbard model by Halboth and Metzner who called it the "Pomeranchuk instability" (PI) of the Fermi surface.[2] Subsequently, several authors studied this problem.[3,4,5,6,7,8,9,10,11,12,13,14,15] It was also argued that the tendency towards a quasi 1D state may enhance a bare anisotropy of the underlying lattice structure, as for example present in $YBa_2Cu_3O_{6+y}$ (YBCO).[13]

Previous studies of the PI for the $t-J$ and the Hubbard models were mainly based on SBMFT and RG methods. Clearly, it is desirable to use an alternative approach, and examine if indeed a PI is present. In this paper, we analyze this problem comprehensively using a variational Monte Carlo (VMC) method.[16,17,18,19] Our VMC results agree qualitatively with previous SBMFT studies over a wide doping range except for discrepancies that show up very close to half-filling. We also supplement the VMC results by presenting results from renormalized mean field theory (RMFT)[20,21] calculations. These results agree well with those from SBMFT, but reveal similar deviations from the VMC results near half-filling. We argue that the disagreement stems from limitations of the mean field theories when dealing with nearly half-filled states.

The outline of the paper is as follows: In Section II, we introduce the $t-J$ Hamiltonian and describe the VMC scheme. The VMC results for a quasi 1D state in an isotropic $t-J$ model are presented in Section III. We discuss the magnitude of asymmetry, the condensation energy per site and the model parameter dependence as a function of the hole concentration (doping). In Section IV, we provide an RMFT study for the PI and give an explicit comparison of the Gutzwiller renormalization scheme (GRS) with the VMC results. Section V is dedicated to a discussion of RMFT and VMC results for the anisotropic $t-J$ model and is followed by our conclusions.

II. MODEL AND VMC SCHEME

We consider the $t-J$ model in two dimensions,

$$H = -\sum_{i,j,\sigma} t_\tau\, c_{i,\sigma}^\dagger c_{j,\sigma} + J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i\, \mathbf{S}_j - \frac{1}{4} n_i n_j \right) , \quad (1)$$

defined in a projected Hilbert space where double occupancies are forbidden. In the above equation, $\mathbf{S}_i$ and n_i are respectively, electron spin and density operators at site i. The kinetic energy is determined by t_τ, the τth neighbor hopping integral. Throughout this paper, we denote nearest neighbor (n.n.) hopping terms by t, and choose next n.n. hopping terms $t' = 0$ or $t' = -0.3t$. For simplicity, we only consider the superexchange coupling $J = 4t^2/U$ between n.n. sites, and choose the value, $J = 0.3t$.

We implement the no-double occupancy constraint in the $t-J$ Hamiltonian by working with Gutzwiller projected states $|\Psi\rangle = P_G\,|\Psi_0\rangle$, where the Gutzwiller projection operator, $P_G = \prod_i (1-n_{i\uparrow}n_{i\downarrow})$. Such wavefunctions were initially proposed as variational states to describe superconductivity in the proximity of a Mott insulating phase.[16,17,20,22] The VMC technique which allows for a numerical evaluation of expectation values in these states successfully predicted $d-$wave pairing in the $t-J$ model.[16,17] The method has been extended more recently to study the coexistence of (and competition between) various phases like antiferromagnetism, flux states, and superconductivity in the $t-J$ model[23,24,25,26]. Motivated by the phenomenology of the high temperature superconductors, other improvements such as the inclusion of longer range hopping terms[27], increase of the number of variational parameters, and introduction of long range correlations through Jastrow factors[28] have also been proposed. Here, we extend previous works by allowing a symmetry breaking between the $x-$ and the $y-$direction in the variational wavefunction $|\Psi\rangle$.

The ground state wave function is written in the form,

$$|\Psi\rangle \;=\; P_G|\Psi_{\rm BCS}\rangle\ , \tag{2}$$

where $|\Psi_{BCS}\rangle \;=\; \left(\sum_k a_k\, c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\right)^{N/2}|0\rangle$ is the N-electron BCS wave function with

$$a_k \;\equiv\; \frac{v_k}{u_k} \;=\; \frac{\Delta_k}{\zeta_k+\sqrt{\zeta_k^2+\Delta_k^2}}\ . \tag{3}$$

To allow for a possible quasi 1D state as well as for finite d- and s-wave pairing, we choose,

$$\begin{aligned}\zeta_k \;=\; &-\;2\,[(1+\delta^{\rm 1D}_{\rm var})\cos k_x+(1-\delta^{\rm 1D}_{\rm var})\cos k_y]\\ &-\;4t'_{\rm var}\cos k_x\cos k_y\;-\;\mu_{\rm var}\end{aligned} \tag{4}$$

and

$$\Delta_k = \Delta^{(d)}_{\rm var}(\cos k_x-\cos k_y)+\Delta^{(s)}_{\rm var}(\cos k_x+\cos k_y)\ . \tag{5}$$

We then have the following five variational parameters: (i) the asymmetry $\delta^{\rm 1D}_{\rm var}$ between n.n. $x-$ and $y-$ hopping matrix elements; (ii) the variational next n.n. hopping term $t'_{\rm var}$; (iii) a variational chemical potential $\mu_{\rm var}$; (iv) and (v) variational parameters for $d-$ and $s-$wave pairing, $\Delta^{(d)}_{\rm var}$ and $\Delta^{(s)}_{\rm var}$, respectively. Using standard VMC techniques[29], we compute energy expectation values and minimize the energy by searching for the optimal set of variational parameters. We use tilted lattices with periodic boundary conditions. Typically, 10^5 Monte Carlo steps are performed for each set of variational parameters. The resulting statistical errors are given in the relevant figures by error bars.

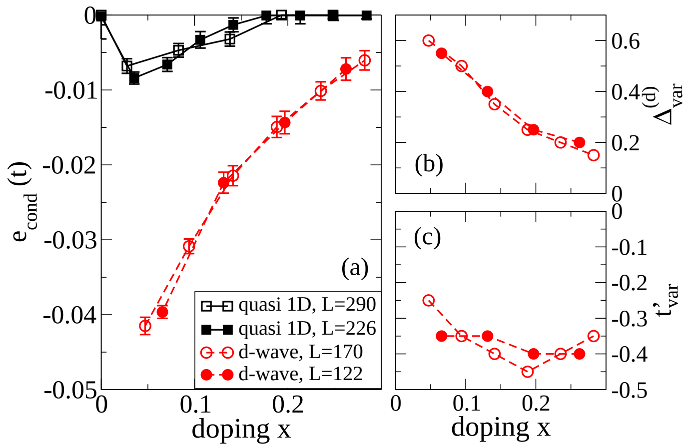

FIG. 1: (color online) (a) VMC results for condensation energies per site $e_{\rm cond}$ of the quasi 1D state ($\Delta_k\equiv 0$) and the d-wave state ($\Delta_k\neq 0$) with $t'=-0.3\,t$. Optimal variational parameters $\Delta^{(d)}_{\rm var}$ and $t'_{\rm var}$ of the d-wave state are shown in (b) and (c). The errors in (b) and (c) are $\Delta\Delta^{(d)}_{\rm var}=0.05$ and $\Delta t'_{\rm var}=0.05$, respectively. System sizes: $L=11^2+1=122$, $L=13^2+1=170$, $L=15^2+1=226$, and $L=17^2+1=290$.

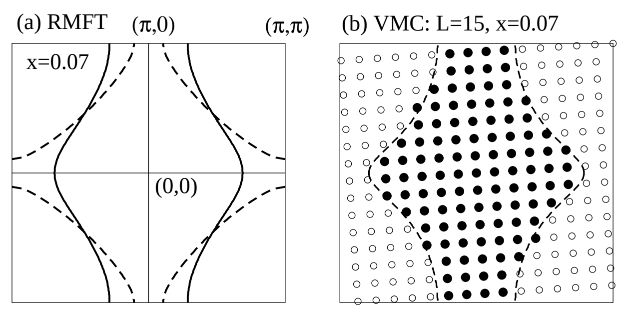

FIG. 2: Fermi surface of the isotropic $t-J$ model with $J=0.3t$ and $t'=-0.3t$ at $x=0.07$ (a) RMFT results for the Fermi surface of the normal state with $\Delta_k\equiv 0$ (solid line) and the optimal d-wave state (dashed line). (b) Best quasi 1D state on a (15^2+1)-sites lattice by VMC; filled circles indicate the Fermi surface.

III. VMC RESULTS FOR THE ISOTROPIC $t-J$ MODEL

We first present results for the isotropic $t-J$ Hamiltonian, with model parameters $J=0.3t$ and $t'=-0.3t$. These are reasonable model parameters for the phenomenology of the high temperature superconductors. The optimal solution for various values of hole concentration, $x=0-0.3$, is determined by searching in the whole variational parameter space. We find that the pure isotropic projected $d-$wave state always optimizes the ground state energy, *i.e.*, the $s-$wave parameter $\Delta^{(s)}_{\rm var}$ and the asymmetry $\delta^{\rm 1D}_{\rm var}$ vanish for all values of x, within our numerical resolution [$\Delta\Delta^{(s)}_{\rm var}=0.05$ and $\Delta\delta^{\rm 1D}_{\rm var}=0.05$].

In Fig. 1(a) (circles) we show the condensation energy per site, $e_{\rm cond}$, of the optimal state with respect to the

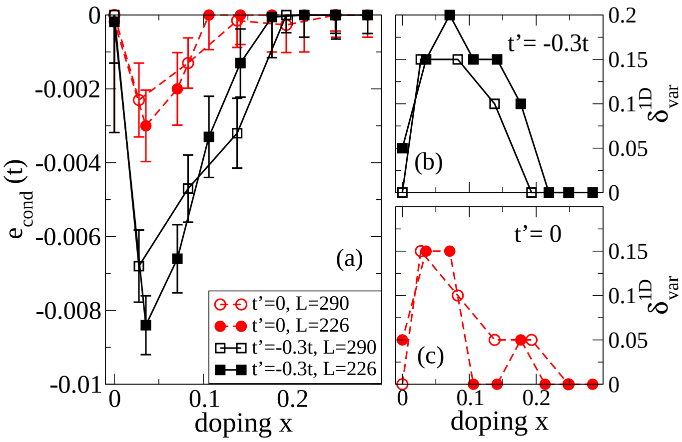

FIG. 3: (color online) VMC results for a quasi 1D state for the isotropic $t-J$ model ($J=0.3t$) with $t'=0$ (circles) and $t'=-0.3t$ (squares). Doping dependence x of (a) the condensation energy per site, e_{cond}, and (b),(c) the optimal variational $\delta_{\text{var}}^{\text{1D}}$. The errors in (b) and (c) are $\Delta\delta_{\text{var}}^{\text{1D}}=0.05$. System sizes: $L=15^2+1=226$ and $L=17^2+1=290$.

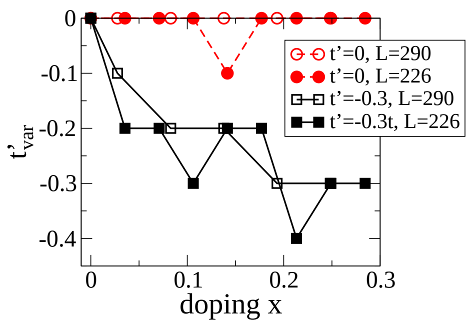

FIG. 4: (color online) VMC results for the quasi 1D state in the isotropic $t-J$ model ($J=0.3t$) with $t'=0$ (circles) and $t'=-0.3t$ (squares). Doping dependence x of the optimal variational t'_{var}. $\Delta t'_{\text{var}}=0.1$; System sizes: $L=15^2+1=226$ and $L=17^2+1=290$.

projected isotropic Fermi sea. The condensation energy, e_{cond}, is calculated by comparing the VMC energy expectation values in the projected Fermi sea and optimal $d-$wave states. We see a continuous increase of $|e_{\text{cond}}|$ and of the superconducting $d-$wave parameter [shown in Fig. 1(b)] as doping x decreases. The optimal variational value for t'_{var} is given in Fig. 1(c). These results show that the additional variational parameters $\Delta_{\text{var}}^{(s)}$ and $\delta_{\text{var}}^{\text{1D}}$ are not relevant for improving the ground state in the isotropic $t-J$ model.

To uncover the PI, it is necessary to suppress superconductivity by setting $\Delta_k \equiv 0$. Doing so, our VMC calculations indeed reveal a PI; we obtain an improvement of the energy expectation value relative to the isotropic projected Fermi sea by using a finite asymmetry $\delta_{\text{var}}^{\text{1D}}$, although the underlying lattice is still isotropic. We compare the condensation energy of this state to that of the $d-$wave state. Results are shown in Fig. 1(a). As for the $d-$wave state, $|e_{\text{cond}}|$ for the quasi 1D state initially increases as x decreases. However its energy gain is much less than that of the $d-$wave, and so the latter is always favored on an isotropic lattice. Furthermore, note that the condensation of the quasi 1D state saturates and finally vanishes very close to half-filling. We will come back to this point later.

The resulting VMC Fermi surface of the optimal quasi 1D state at $x=0.07$ is shown in Fig. 2(b). It reveals why finite size effects become important in the VMC calculations when dealing with a finite asymmetry in the projected Fermi sea. Varying $\delta_{\text{var}}^{\text{1D}}$ causes discontinuous changes of the Fermi surface on a finite lattice. The occupied states regroup for certain $\delta_{\text{var}}^{\text{1D}}$ leading to small yet discontinuous changes in the FS as a function of the variational parameter $\delta_{\text{var}}^{\text{1D}}$.

These finite size effects cause a rather large error for the optimal value of asymmetry, $\Delta\delta_{\text{var}}^{\text{1D}}=0.05$, and for the effective next n.n. hopping, $\Delta t'_{\text{var}}=0.05-0.1$. The jump size increases with decreasing system size, thus requiring sufficiently large lattices. The problem is less severe when considering a superconducting state, where the occupancy in momentum space changes continuously at the Fermi surface.

To consider the effect of t' on the PI, we compared the two cases, $t'=0$ and $t'=-0.3t$, in the absence of superconducting order ($\Delta_k \equiv 0$). The PI is stronger for $t'<0$, yielding a larger condensation energy [Fig. 3(a)]. As seen in Fig. 3(b), the anisotropy is significant even at higher doping levels and exists up to $x \approx 0.2$ for $t'=-0.3t$. For $t'=0$, the $\delta_{\text{var}}^{\text{1D}}$ is significant only in the range, $x=0.03-0.10$ [Fig. 3(c)]. In Fig. 4 we show the optimal variational value for t'_{var}. Interestingly, $t'_{\text{var}} \to 0$ for $x \to 0$ even for a bare dispersion $t'=-0.3t$. Recently, we reported a similar renormalization of the next n.n. hopping terms due to strong coupling effects within RMFT.[21,30]

Although there is good overall agreement between our VMC data and SBMFT results, we find clear and significant discrepancies in the limit $x \to 0$. As seen in Fig. 3(a)-(c) the asymmetry goes to zero at $x=0$ within our VMC calculations. On the other hand, SBMFT as well as RMFT (discussed in the next section) predict a pure 1D state at half-filling when $\Delta_k \equiv 0$. This hints at limitations of the mean field theories when treating states near half-filling. We shall discuss this in more detail, after discussing results from the RMFT calculation for the PI.

IV. RMFT AND GUTZWILLER RENORMALIZATION FOR THE ISOTROPIC $t-J$ MODEL

In this section, we present some results from renormalized mean field theory (RMFT). The RMFT gap equations have been derived in previous works[20,21]. Here, we solve them allowing for possible anisotropic solutions.

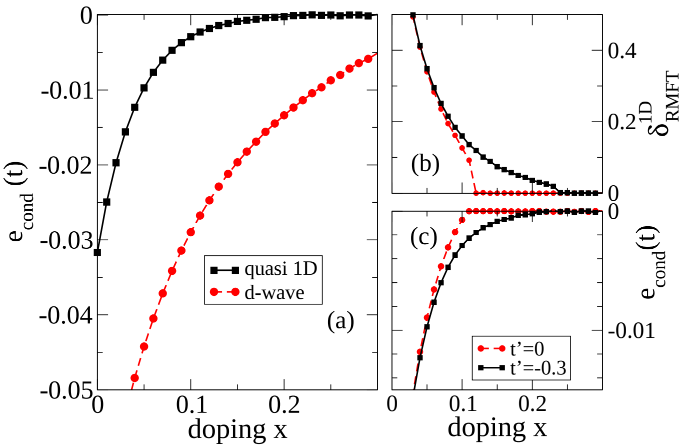

FIG. 5: (color online) RMFT results for the isotropic $t-J$ model with $J = 0.3t$. (a) Condensation energy per site relative to the isotropic non-SC solution ($\Delta_k \equiv 0$, $\xi_x = \xi_y$) for the quasi 1D state ($\Delta_\tau \equiv 0$) and for the optimal d-wave state with $t' = -0.3t$. (b) Asymmetry and (c) condensation energy per site for the quasi 1D state with $t' = 0$ and $t' = -0.3$, respectively.

We find that the optimal self consistent state remains a pure d-wave superconductor. This is consistent with the VMC data presented in the previous section, and with SBMFT calculations.[1] The condensation energy of this optimal state relative to the isotropic renormalized Fermi sea is shown in Fig. 5. To uncover the PI, we now look for solutions with the constraint $\Delta_k \equiv 0$, as before. Doing so, we find two self consistent solutions for sufficiently small doping: an isotropic and an anisotropic renormalized Fermi sea. We compare the condensation energy of the anisotropic quasi 1D state with that of the d-wave pairing state for a bare dispersion $t' = -0.3t$. As seen from Fig. 5(a), the doping dependence as well as the magnitude of the condensation energy agree well with the VMC results in Fig. 1(a). However, the two results begin to differ in the vicinity of $x = 0$, where the condensation energy of the quasi 1D state vanishes in the VMC scheme.

Within RMFT, the order parameter characterizing the asymmetry, $\delta^{1D}_{\rm RMFT}$ is given by,

$$\delta^{1D}_{\rm RMFT} \equiv \frac{\tilde{t}_x - \tilde{t}_y}{\tilde{t}_x + \tilde{t}_y} \; . \tag{6}$$

Here, the effective hopping $\tilde{t}_\tau$ in the τ-direction is related to the bare hopping t_τ by[31],

$$\tilde{t}_\tau \equiv g_t \, t_\tau + \frac{3g_s - 1}{8} J \, \xi_\tau \; , \tag{7}$$

where $J = 4t_\tau^2/U$, $\xi_\tau \equiv \sum_\sigma \langle c^\dagger_{i,\sigma} c_{i+\tau,\sigma}\rangle_{|\Psi_0\rangle}$, and $\tau = x, y$. The renormalization factors for the kinetic energy, $g_t = 2x/(1+x)$, and for the spin-spin correlation, $g_s = 4/(1+x)^2$, are derived within the Gutzwiller Renormalization Scheme (GRS).

The origin of the PI can be seen directly from Eq. (7). It shows that the tendency to a quasi 1D state stems from the J-term [2nd term in Eq. (7)] because it includes the factor ξ_τ. For an isotropic dispersion it is the only quantity in Eq. (7) that may cause an anisotropy in the effective hopping $\tilde{t}_\tau$. Similar arguments apply for the enhancement of a bare asymmetry δ^{1D}_0 in a slightly anisotropic lattice (see also discussion below). The origin of the PI may also be understood in the framework of a Landau-Ginzburg analysis as shown by Yamase and Kohno within SBMFT.[1]

In Fig. 5(b) and (c), we show our results for $\delta^{1D}_{\rm RMFT}$ and the condensation energy relative to the projected (symmetric) Fermi sea. Results are shown as a function of x for two values of t', $t' = 0$ and $t' = -0.3t$. We see that a negative t' favors the PI, in agreement with SBMFT and VMC results. The asymmetry $\delta^{1D}_{\rm RMFT}$ is shown in Fig. 5(b) and agrees quantitatively with the VMC results in Fig. 3(b),(c) for $x > 0.07$. However, for $x \to 0$ the asymmetry increases strongly within RMFT, whereas it saturates and finally disappears within the VMC scheme.

The Fermi surface of the quasi 1D state from RMFT at $x = 0.07$ is shown in Fig. 2(a) and agrees well with that obtained from VMC calculations for the same doping [Fig. 2(b)].

We now turn our attention to the discrepancy between VMC and RMFT (and SBMFT) results near half-filling. In Fig. 6, we plot the kinetic energy $E_{\rm kin}$ and the superexchange energy E_J (J-term in the Hamiltonian) for the projected Fermi Sea ($\Delta_k \equiv 0$) as a function of the asymmetry $\delta^{1D}_{\rm var}$ for various doping concentrations. We compare the VMC data with the results from the Gutzwiller renormalization scheme (GRS) for $t' = 0$. Fig. 6 shows that the GRS only approximately agrees with the nearly exact VMC results. In particular, the behavior of the superexchange energy as a function of $\delta^{1D}_{\rm var}$ is qualitatively different in the two schemes. The discrepancies are acute near half filling (see data for $x = 0$ and $x = 0.035$). A reasonable agreement is obtained for larger doping. In general, the VMC data shows a weaker dependence of the energy on the asymmetry $\delta^{1D}_{\rm var}$.

Our VMC results are also consistent with previous studies of the Gutzwiller wavefunction at half-filling in the 1D limit[32], which corresponds to $\delta^{1D}_{\rm var} \equiv 1$ in our calculations. The superexchange energy (deduced from the n.n. spin-spin correlations) of the pure 1D state on an isotropic 2D lattice is much worse than that of the projected isotropic 2D Fermi sea. On the contrary a simple evaluation by the GRS would favor a pure 1D state at half-filling. We thus think that the drawbacks of the mean field theories partially stem from invoking 1D physics by allowing a finite asymmetry. We further note that the renormalization effects become largest near half-filling. Therefore, it is naturally that discrepancies can show up in this limit, as already seen in previous VMC studies, e.g., for the quasiparticle weight renormalization[33,34,35,36]. With that in mind, our VMC

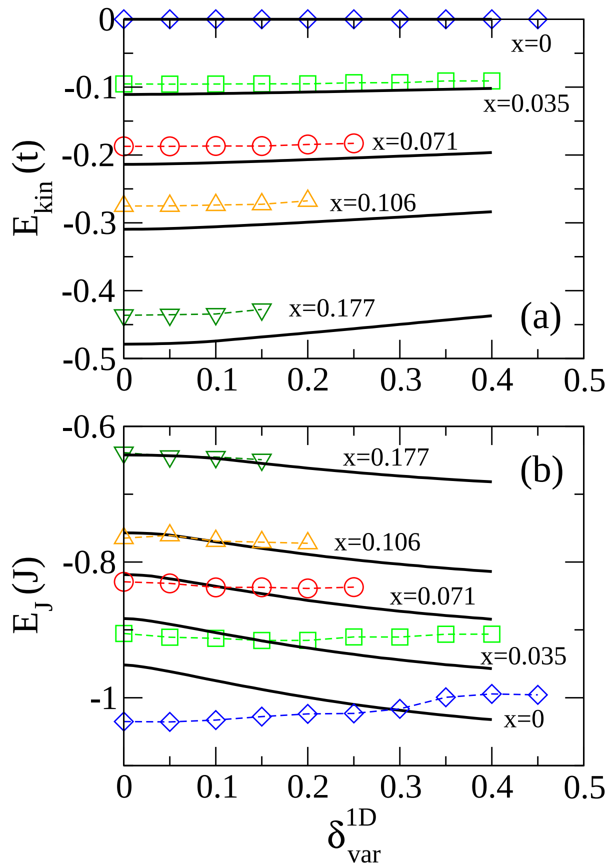

FIG. 6: (color online) Comparison of the Gutzwiller renormalization scheme (GRS, solid lines) and VMC results (dashed lines with symbols) for (a) the kinetic and (b) the superexchange energy of the projected Fermi Sea ($\Delta_k \equiv 0$) at different doping levels x. The dependence on the asymmetry $\delta^{1D}_{\rm var}$ is illustrated. VMC results are taken from the $L = 15^2 + 1$-system and $t' = 0$. Statistical VMC errors are much smaller than the symbol size.

results are not really surprising. Though the GRS gives valuable insights into the behavior of strongly correlated electronic systems, the above results show that a verification of GRS results by the VMC technique is often very important. These limitations of the GRS directly impact the RMFT (which is based on the GRS) and the SBMFT (which is closely related to RMFT).

V. RMFT AND VMC CALCULATIONS FOR THE ANISOTROPIC $t - J$ MODEL

Our results from VMC and RMFT confirm that a quasi 1D state is always suppressed by the d-wave pairing state. A PI occurs only when $\Delta_k \equiv 0$. However, the situation can be quite different when the underlying lattice structure is anisotropic. In this case, the tendency towards a quasi 1D state is present even in the superconducting state. SBMFT[1] predicts an optimal state which has a dominant d-wave symmetry with a small s-wave

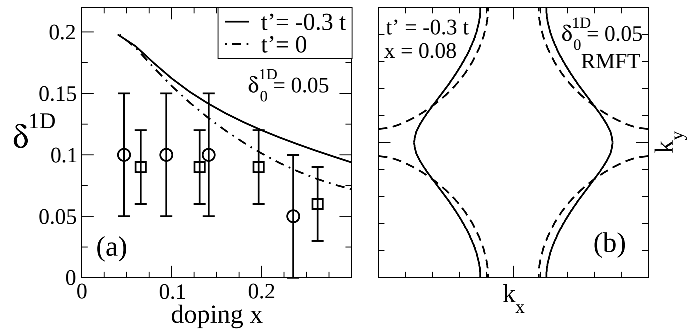

FIG. 7: RMFT and VMC results for the $d + s$-wave ground state of the anisotropic $t - J$ model with $J = 0.3t$ and $\delta^{1D}_0 \equiv (t_x - t_y)/(t_x + t_y) = 0.05$. (a) Effective asymmetry $\delta^{1D} \equiv (\tilde{t}_x - \tilde{t}_y)/(\tilde{t}_x + \tilde{t}_y)$ from RMFT as a function of hole doping x for (dashed) $t' = 0$ and (solid) $t' = -0.3t$. VMC results for $t' = 0$ are given by squares and circles for $L = 122$ and $L = 170$, respectively. (b) RMFT Fermi surface (solid lines) of the $d+s$-wave ground state and the tight binding dispersion (dashed) at $x = 0.08$ with $t' = -0.3t$ and $\delta^0_{1D} = 0.025$.

contribution.[37] Interestingly, the bare anisotropy δ^{1D}_0 of the lattice is enhanced due to the electron correlations. Here we re-examine this prediction within the RMFT and VMC schemes. Results from RMFT are shown in Fig. 7(a) and (b) and agree quantitatively with the SBMFT data. As seen in Fig. 7(a), the bare asymmetry of $\delta^{1D}_0 = 0.05$ increases within the RMFT calculations up to about $\delta^{1D}_{\rm opt} = 0.2$ in the underdoped regime. These results are confirmed to some extent by VMC calculations for $t' = 0$ in Fig. 7(a) (circles and squares), that show an increase of the asymmetry up to about $\delta^{1D}_{\rm var} \approx 0.1$. However, owing to numerical difficulties, the errors in these VMC calculations are quite large.[38] In Fig. 7(b), we compare the Fermi surface obtained from the bare dispersion ($\delta^{1D}_0 = 0.05$) with that of the optimal superconducting state obtained by solving the RMFT equations self consistently, for $x = 0.08$. As seen in the figure, the enhancement of anisotropy due to strong correlations may even lead to a change in the topology of the underlying Fermi surface.

VI. CONCLUSIONS

In this paper, we performed a Variational Monte Carlo (VMC) study of the Pomeranchuk instability in the isotropic $t - J$ model. We also supplemented the study with results from renormalized mean field theory (RMFT). Our results are in agreement with earlier calculations from slave boson mean field theory (SBMFT) and exact diagonaliziation on small clusters[8] and show that the instability is uncovered when the (optimal) d-wave superconducting state is suppressed. The Pomeranchuk instability is seen for values of hole concentration between $x \approx 0.03$ and $x \approx 0.20$, depending on the magnitude of the next n.n. hopping integral t'. We find that a small

bare asymmetry δ_0^{1D} is enhanced within an anisotropic $t-J$ model even in the superconducting state. Although there is good overall agreement between the VMC calculations and results from RMFT and SBMFT, discrepancies arise very close to half-filling, showing the limitations of these mean field theories in this regime. This underlines the importance of complementary VMC studies to confirm or disprove the results from RMFT or SBMFT calculations.

The tendency towards a quasi one dimensional state in a strongly correlated electron systems is mainly governed by the superexchange J. Since $J \propto 4t^2/U$, a small asymmetry in the bare hopping integral t becomes twice as large in the superexchange energy. Hence, it is natural that the effects discussed in this paper are largest in the underdoped regime, where the dispersion is mainly determined by J. The tendency towards a quasi one dimensional state may be also enhanced if phonons are coupled to the lattice. The influence of such dynamic effects should be clarified in future studies.

Acknowledgments

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